

Product Name: Vismodegib

Catalog No.: 7710

Batch No.: 1

CAS Number: 879085-55-9

IUPAC Name: 2-Chloro-*N*-[4-chloro-3-(2-pyridinyl)phenyl]-4-(methylsulfonyl)benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₉H₁₄Cl₂N₂O₃S.

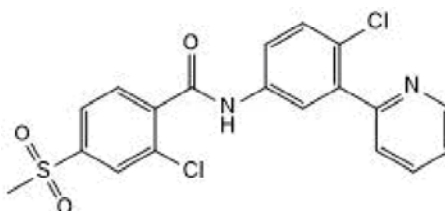
Batch Molecular Weight: 421.3

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	54.17	3.35	6.65
Found	53.92	3.31	6.59

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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CAS Number: 879085-55-9

IUPAC Name: 2-Chloro-N-[4-chloro-3-(2-pyridinyl)phenyl]-4-(methylsulfonyl)benzamide

Description:

Vismodegib is a potent hedgehog pathway inhibitor (IC₅₀ = 3 nM). It causes tumor regressions in allograft medulloblastoma mice model and tumor growth inhibition in a xenograft mouse models of colorectal cancer. Vismodegib is orally bioavailable.

Physical and Chemical Properties:

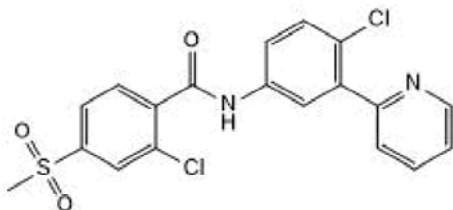
Batch Molecular Formula: C₁₉H₁₄Cl₂N₂O₃S.

Batch Molecular Weight: 421.3

Physical Appearance: Pale yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Wong et al (2011) Pharmacokinetic-pharmacodynamic analysis of vismodegib in preclinical models of mutational and ligand-dependent Hedgehog pathway activation. *Clin.Cancer Res.* **17** 4682. PMID: 21610148.

Robarge et al (2009) GDC-0449-a potent inhibitor of the hedgehog pathway. *Bioorg.Med.Chem.Lett.* **19** 5576. PMID: 19716296.

Wong et al (2009) Preclinical assessment of the absorption, distribution, metabolism and excretion of GDC-0449 (2-chloro-N-(4-chloro-3-(pyridin-2-yl)phenyl)-4-(methylsulfonyl)benzamide), an orally bioavailable systemic Hedgehog signalling pathway inhibitor. *Xenobiotica* **39** 850. PMID: 19845436.

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